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Causal Graph Transformer for Treatment Effect Estimation Under Unknown Interference

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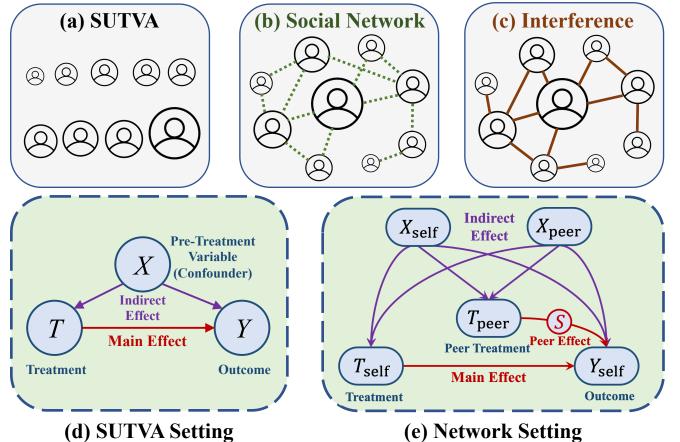


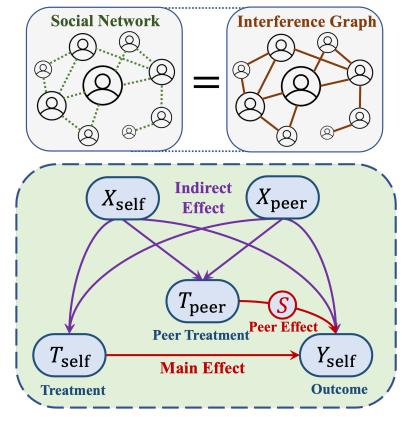


Treatment Effect Estimation Under Unknown Interference.

Stable Unit Treatment Value Assumption (SUTVA) has two main components:

- No Interference: Each individual's potential outcome is only influenced by their own treatment status and not by the treatment status of others.
- No Hidden Versions of Treatment: Each treatment has a single, consistent version without variation.



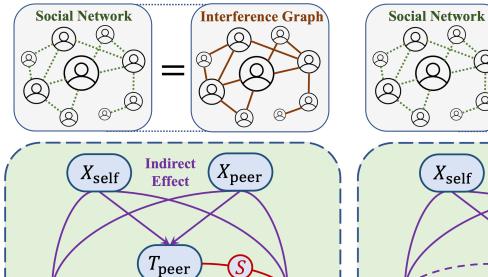


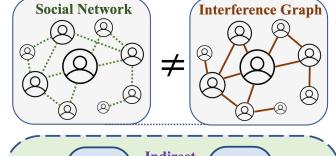


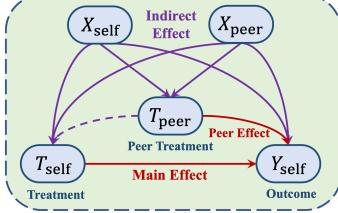
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(a) Traditional Network Setting

Main Effect

 $T_{\rm self}$

Peer Treatment Peer Effect

 Y_{self}

(b) General Network Setting

Different from Traditional Network Settings

- 1. The interference graph is not the same as the social network; the networked interference structure is unknown.
- 2. The structural function describing the effect of peer treatments (T_{peer}) on self-outcomes (Y_{self}), also known as the summary/aggregation function of exposure mapping, is unknown.
- 3. In the general network setting, there may be potential causal effects between peer treatments (T_{peer}) and self-treatments (T_{self}).



Representative Algorithms on Observational Networked Data.

	Sett	ings	1	Effects	S	I	Prior		Sub-Modules	
Method	Interference	Unmeasured	Main	Peer	Total	Graph	Summary	Reweighting	Representation	Attention
CNE (Veitch et al., 2019)		P	√			✓		✓		
NetDeconf (Guo et al., 2020)		P	✓			✓			\checkmark	
DRLearner (Leung & Loupos, 2022)	✓		✓	\checkmark	\checkmark	✓		✓		
SPNet (Huang et al., 2023)	√	P	√			✓		✓	\checkmark	\checkmark
Net-TMLE (Ogburn et al., 2024)	√		✓			✓	\checkmark	✓		
GDML (Khatami et al., 2024)	√		✓	\checkmark	\	✓	\checkmark	✓		
G-HSIC (Ma & Tresp, 2021)	√		✓			√	\checkmark		\checkmark	
RRNet (Cai et al., 2023)	√		✓	\checkmark	√	✓	\checkmark	✓	\checkmark	
NetEst (Jiang & Sun, 2022)	√		✓	\checkmark	\checkmark	√	\checkmark		\checkmark	
Uncertainty (Bhattacharya et al., 2020)	√				√					
UNITE (Lin et al., 2024)	✓		✓						\checkmark	
CauGramer (Ours)	\checkmark	✓	√	\checkmark	\checkmark				\checkmark	✓

- Without interference effects: CNE and NetDeconf algorithms use reweighting and balanced representation learning;
- Known interference graph: DRLearner, SPNet, Net-TMLE, GDML, G-HSIC, RRNet, NetEst;
- Unknown interference:
 - Uncertainty algorithm proposes a method integrating structure learning and causal inference to estimate the Population Average Overall Effect (PAOE) under network uncertainty and partial interference.
 - UNITE algorithm uses a Graph Structure Learner to infer the hidden interference structure by constructing a complete graph and imposing L0-norm regularization to identify significant connections.





Parameters of Interest.

Definition 1 (Individual Main Effects (IME)). *IME denotes the effects of self-treatment, i.e.*, $\tau_{IME}(\boldsymbol{x}_i) = y(\boldsymbol{x}_i, \boldsymbol{x}_{\mathcal{P}_i}, 1, \boldsymbol{0}_{\mathcal{P}}) - y(\boldsymbol{x}_i, \boldsymbol{x}_{\mathcal{P}_i}, 0, \boldsymbol{0}_{\mathcal{P}}).$

Definition 2 (Individual Peer Effects (IPE)). *IPE denotes the effects of peers' treatments, i.e.*, $\tau_{IPE}(\boldsymbol{x}_i, \boldsymbol{t}_{\mathcal{P}}) = y(\boldsymbol{x}_i, \boldsymbol{x}_{\mathcal{P}_i}, 0, \boldsymbol{t}_{\mathcal{P}}) - y(\boldsymbol{x}_i, \boldsymbol{x}_{\mathcal{P}_i}, 0, \boldsymbol{0}_{\mathcal{P}})$ for any $\boldsymbol{t}_{\mathcal{P}} \in \mathcal{T}^{|\mathcal{P}_i|}$.

Definition 3 (Individual Total Effects (ITE)). *ITE denotes the combination of main and peer effects,* i.e., $\tau_{ITE}(\boldsymbol{x}_i, \boldsymbol{t}_{\mathcal{P}}) = y(\boldsymbol{x}_i, \boldsymbol{x}_{\mathcal{P}_i}, 1, \boldsymbol{t}_{\mathcal{P}}) - y(\boldsymbol{x}_i, \boldsymbol{x}_{\mathcal{P}_i}, 0, \boldsymbol{0}_{\mathcal{P}})$ for any $\boldsymbol{t}_{\mathcal{P}} \in \mathcal{T}^{|\mathcal{P}_i|}$.

Identification Assumptions.

To precisely estimate the three treatment effects, i.e., ME, PE, and TE, we first discuss causal identification under the standard causal assumptions on networked data (Jiang & Sun, 2022).

Assumption 1 (Positivity). The probability of a unit with their peers to receive any treatment pair $(t, \mathbf{t}_{\mathcal{P}})$ is always positive, i.e., $0 < \mathbb{P}(t_i = t, \mathbf{t}_{\mathcal{P}_i} = \mathbf{t}_{\mathcal{P}} \mid \mathbf{x}_i, \mathbf{x}_{\mathcal{P}_i}) < 1$ for any \mathbf{x}_i .

Assumption 2 (Consistency). The potential outcome is the same as the observed outcome under the same self-treatment and peer-treatments, i.e., $y_i = y(\mathbf{x}_i, \mathbf{x}_{\mathcal{P}_i}, t_i, \mathbf{t}_{\mathcal{P}_i})$ for treatment pair $(t_i, \mathbf{t}_{\mathcal{P}_i})$.

Assumption 3 (Unconfoundedness). The self-treatment and peer-treatments are independent of the potential outcome given self and peer' features, i.e., $y(\mathbf{x}_i, \mathbf{x}_{\mathcal{P}_i}, t, \mathbf{t}_{\mathcal{P}}) \perp (t, \mathbf{t}_{\mathcal{P}}) \mid (\mathbf{x}_i, \mathbf{x}_{\mathcal{P}_i})$.

Methods



Identification Theorems.

Theorem 1 (Causal Identification). Given these assumptions, while the Stable Unit Treatment Value Assumption (SUTVA) does not hold under networked interference, the treatment effects are identified as long as we can control the confounders x_i and the peers $x_{\mathcal{P}_i}$.

Proof. As shown in Figure 1, when we consider the (unknown) peer interference graph, all common causes $(x_i, x_{\mathcal{P}_i})$ of treatment pair $(t_i, t_{\mathcal{P}_i})$ and outcomes y_i have been discovered. Thus, we have:

$$\tau_{\text{ITE}}(\boldsymbol{x}_{i}, \boldsymbol{t}_{\mathcal{P}}) = \mathbb{E}[y(\boldsymbol{x}_{i}, \boldsymbol{x}_{\mathcal{P}_{i}}, 1, \boldsymbol{t}_{\mathcal{P}}) \mid \boldsymbol{x}_{i}, \boldsymbol{x}_{\mathcal{P}_{i}}] - \mathbb{E}[y(\boldsymbol{x}_{i}, \boldsymbol{x}_{\mathcal{P}_{i}}, 0, \boldsymbol{0}_{\mathcal{P}}) \mid \boldsymbol{x}_{i}, \boldsymbol{x}_{\mathcal{P}_{i}}] \\
= \mathbb{E}[y(\boldsymbol{x}_{i}, \boldsymbol{x}_{\mathcal{P}_{i}}, 1, \boldsymbol{t}_{\mathcal{P}}) \mid \boldsymbol{x}_{i}, \boldsymbol{x}_{\mathcal{P}_{i}}, t, \boldsymbol{t}_{\mathcal{P}}] - \mathbb{E}[y(\boldsymbol{x}_{i}, \boldsymbol{x}_{\mathcal{P}_{i}}, 0, \boldsymbol{0}_{\mathcal{P}}) \mid \boldsymbol{x}_{i}, \boldsymbol{x}_{\mathcal{P}_{i}}, 0, \boldsymbol{0}_{\mathcal{P}}] \\
= \mathbb{E}[y_{1, \boldsymbol{t}_{\mathcal{P}}} \mid \boldsymbol{x}_{i}, \boldsymbol{x}_{\mathcal{P}_{i}}, t, \boldsymbol{t}_{\mathcal{P}}] - \mathbb{E}[y_{0, \boldsymbol{0}_{\mathcal{P}}} \mid \boldsymbol{x}_{i}, \boldsymbol{x}_{\mathcal{P}_{i}}, 0, \boldsymbol{0}_{\mathcal{P}}], \tag{2}$$

where y_{t,t_p} is the observed outcome when the unit and its peers have features x_i, x_{p_i} and receive the treatment pair (t, t_P) . Eq. (1) holds under the Uncounfoundedness, i.e., $y(x_i, x_{P_i}, t, t_P) \perp (t, t_P)$ $(x_i, x_{\mathcal{P}_i})$. Eq. (2) holds under the Consistency Assumption, i.e., $y_{t,t_{\mathcal{P}}} = y(x_i, x_{\mathcal{P}_i}, t, t_{\mathcal{P}})$. Theorem 1 holds for any treatment pair (t, t_P) under Positivity Assumption, i.e., $\mathbb{P}(t_i = t, t_{P_i} = t_P) > 0$. \square

However, since the interference graph is unknown, we cannot directly model the expectation function $\mathbb{E}[y_{t,t_{\mathcal{P}}} \mid x_i, x_{\mathcal{P}_i}, t, t_{\mathcal{P}}]$. Nevertheless, under the Unconfoundedness assumption, we know that $y(x_i, x_{\mathcal{P}_i}, t, t_{\mathcal{P}}) \perp \{t_i, t_{\mathcal{P}_i}\} \mid \{x_i, x_{\mathcal{P}_i}\}$. Therefore, if we control for all observed confounders $\{x_i\}_{i=1}^n$, we can infer to $y(x_i, x_{\mathcal{P}_i}, t, t_{\mathcal{P}}) \perp \{t_i, t_{\mathcal{P}_i}\} \mid \{x_i\}_{i=1}^n$. The interaction information in the interference graph is embedded within the node and network features. To capture this, we propose using two functions, g_x and g_t , to represent peer feature and peer treatment information, respectively.





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= \mathbb{E}[y(\boldsymbol{x}_{i}, \boldsymbol{x}_{\mathcal{P}_{i}}, 1, \boldsymbol{t}_{\mathcal{P}}) \mid \boldsymbol{x}_{i}, \boldsymbol{x}_{\mathcal{P}_{i}}, t, \boldsymbol{t}_{\mathcal{P}}] - \mathbb{E}[y(\boldsymbol{x}_{i}, \boldsymbol{x}_{\mathcal{P}_{i}}, 0, \boldsymbol{0}_{\mathcal{P}}) \mid \boldsymbol{x}_{i}, \boldsymbol{x}_{\mathcal{P}_{i}}, 0, \boldsymbol{0}_{\mathcal{P}}] \\
= \mathbb{E}[y_{1, \boldsymbol{t}_{\mathcal{P}}} \mid \boldsymbol{x}_{i}, \boldsymbol{x}_{\mathcal{P}_{i}}, t, \boldsymbol{t}_{\mathcal{P}}] - \mathbb{E}[y_{0, \boldsymbol{0}_{\mathcal{P}}} \mid \boldsymbol{x}_{i}, \boldsymbol{x}_{\mathcal{P}_{i}}, 0, \boldsymbol{0}_{\mathcal{P}}], \tag{2}$$

where $y_{t,t_{\mathcal{P}}}$ is the observed outcome when the unit and its peers have features $\boldsymbol{x}_i, \boldsymbol{x}_{\mathcal{P}_i}$ and receive the treatment pair $(t, \boldsymbol{t}_{\mathcal{P}})$. Eq. (1) holds under the Uncounfoundedness, i.e., $y(\boldsymbol{x}_i, \boldsymbol{x}_{\mathcal{P}_i}, t, \boldsymbol{t}_{\mathcal{P}}) \perp \!\!\! \perp (t, \boldsymbol{t}_{\mathcal{P}}) \mid (\boldsymbol{x}_i, \boldsymbol{x}_{\mathcal{P}_i})$. Eq. (2) holds under the Consistency Assumption, i.e., $y_{t,t_{\mathcal{P}}} = y(\boldsymbol{x}_i, \boldsymbol{x}_{\mathcal{P}_i}, t, \boldsymbol{t}_{\mathcal{P}})$. Theorem 1 holds for any treatment pair $(t, \boldsymbol{t}_{\mathcal{P}})$ under Positivity Assumption, i.e., $\mathbb{P}(t_i = t, \boldsymbol{t}_{\mathcal{P}_i} = \boldsymbol{t}_{\mathcal{P}}) > 0$. \square

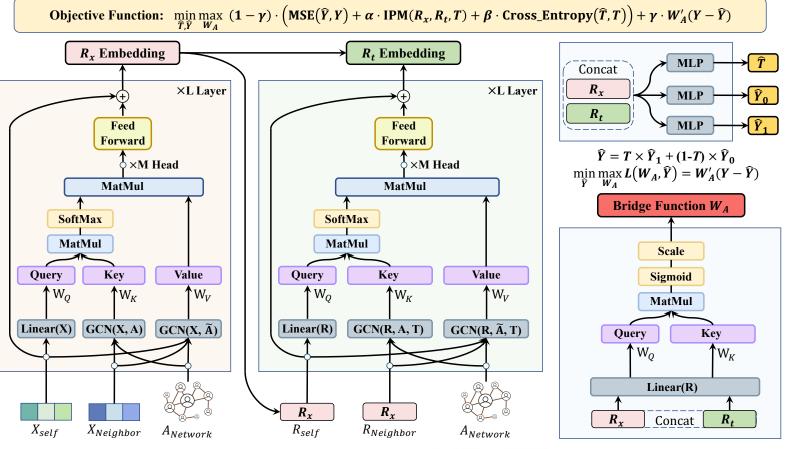
Assumption 4 (Representation). The treatment vector $\mathbf{t}_{\mathcal{P}_i}$ of peer nodes can be captured by a peer treatment function g_t , and the confounder vector $\mathbf{x}_{\mathcal{P}_i}$ by a peer confounder function g_x .

Proposition 1 (Interference). *If the unknown interference graph* E *is latent in full graph information* $\{x, t, A\}$ *, then, the outcome* $\mathbb{E}[y_{t,t_{\mathcal{P}}} \mid x_i, x_{\mathcal{P}_i}, t, t_{\mathcal{P}}]$ *is identified.*





Causality-based Graph Transformer (CauGramer)



Advance: Graph Transformer

Methods

This paper designs a causalitybased graph transformer that models network interference by constructing linear queries from individual features, graph convolutional keys from peer features, and combined values. This approach expands the receptive field of the graph neural network while capturing complex interference patterns.

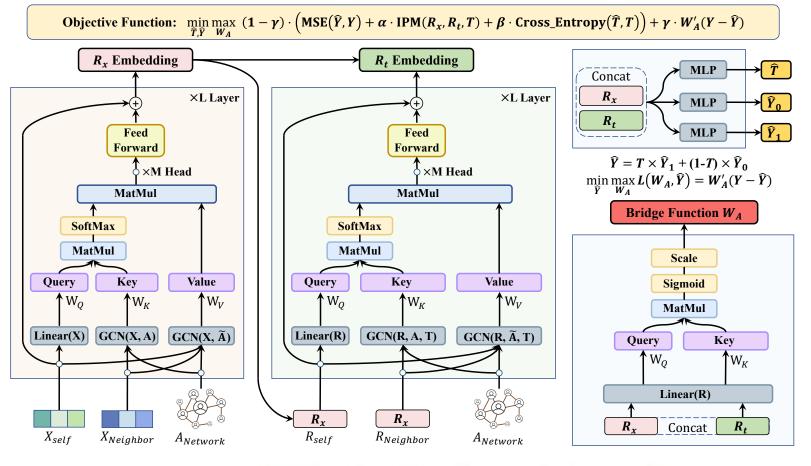
$$\boldsymbol{r}_{x}^{(h+1)} = \operatorname{Attention}_{x}^{(h)} \cdot \mathbf{V}_{x}^{(h)} = \operatorname{Softmax}\left(\frac{\mathbf{Q}_{x}^{(h)} \cdot \mathbf{K}_{x}^{(h)\prime}}{\sqrt{d}}\right) \cdot \mathbf{V}_{x}^{(h)}, \tag{4}$$

$$Q_x^{(h)} = \text{Linear}_x^{(h)}(\mathbf{r}_x^{(h)})W_Q^{(h)\prime}, \quad K_x^{(h)} = \text{GCN}_{xk}^{(h)}(\mathbf{r}_x^{(h)}, \mathbf{A})W_K^{(h)\prime}, \quad V_x^{(h)} = \text{GCN}_{xv}^{(h)}(\mathbf{r}_x^{(h)}, \tilde{\mathbf{A}})W_V^{(h)\prime}. \quad (5)$$





Causality-based Graph Transformer (CauGramer)



Advance: Joint Balancing

Traditional algorithms assume that peer-treatments would not influent self-treatment, only address the confounding bias in main effect estimation.

In this work, we proposes a joint representation balancing, which relaxes the previous treatmentindependence assumption.

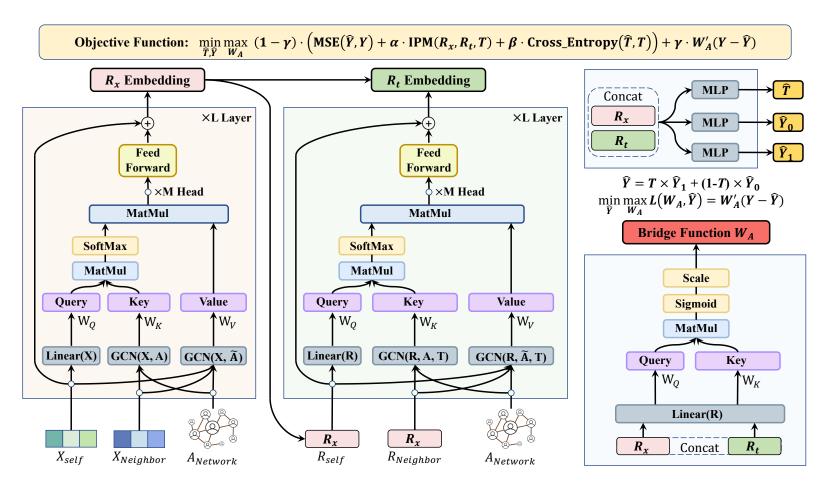
$$IPM(r, t) = Wass(\{r_{i:t_i=0}\}, \{r_{j:t_j=1}\}),$$

Cross_Entropy(
$$\hat{t}, t$$
) = $-\frac{1}{N} \sum_{i=1}^{N} [t_i \log (p_i) + (1 - t_i) \log (1 - p_i)],$

$$\mathcal{L}_y = \text{MSE}(\hat{\boldsymbol{y}}, \boldsymbol{y}) + \alpha \cdot \text{IPM}(\boldsymbol{r}, \boldsymbol{t}) + \beta \cdot \text{Cross_Entropy}(\hat{\boldsymbol{t}}, \boldsymbol{t}),$$



Causality-based Graph Transformer (CauGramer)



Advance: Minimax Constraint

Methods

We refine the potential outcome prediction model using a minimax moment constraint, enabling it to correct for confounding bias through bridge function, even in the presence of unmeasured confounders.

$$y^* = \underset{\hat{\boldsymbol{y}}}{\operatorname{arg \, min}} \max_{q \in \mathbb{Q}} \mathbb{E}[(\boldsymbol{y} - \hat{\boldsymbol{y}})q(\boldsymbol{r}, \boldsymbol{t})], \quad q(\boldsymbol{r}, \boldsymbol{t}) = \operatorname{Sigmoid}(\mathbf{Q} \cdot \mathbf{K}'),$$
 (11)

Experiment Results

Datasets.

Following previous works, we use pseudo-real datasets from BlogCatalog (BC) and Flickr, where the features (x) and social networks (A) are real, while treatments (t), outcomes (y), and interference (E) are simulated.

Evaluation.

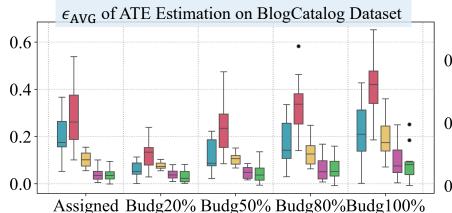
We use the Average Absolute Error (ϵ_{AVG}) on AME, APE, and ATE as evaluation metric We use ($\sqrt{\epsilon_{PEHE}}$) on IME, IPE, and ITE as evaluation metric.

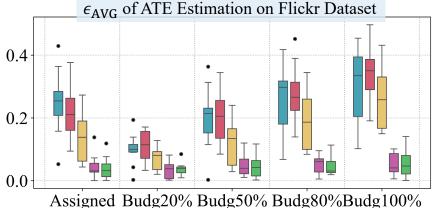
Table 2: Results of Constant Treatment Effects Estimation on BlogCatalog (BC) and Flickr Datasets.

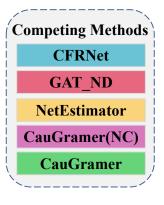
BC	Effects	CFRNet	DRLearner	NetDeconf	G-HSIC	SPNet	CAL	Graphormer	RRNet	NetEst	CauGramer
$\epsilon_{ ext{AVE}}$	APE	$0.117_{\pm 0.06}$	$0.207_{\pm 0.02}$	$0.351_{\pm 0.09}$	$0.387_{\pm0.02}$	$0.223_{\pm0.10}$	$0.370_{\pm 0.07}$	$0.086_{\pm 0.06} \\ 0.436_{\pm 0.03} \\ 0.349_{\pm 0.07}$	$0.229_{\pm 0.06}$	$0.078_{\pm 0.02}$	$0.034_{\pm 0.03}$
$\sqrt{\epsilon_{ m PEHE}}$	IPE	$0.122_{\pm 0.06}$	$0.220_{\pm 0.02}$	$0.365_{\pm0.09}$	$0.410_{\pm 0.03}$	$0.230_{\pm 0.10}$	$0.384_{\pm 0.07}$	$\begin{array}{c} 0.211_{\pm 0.09} \\ 0.457_{\pm 0.03} \\ 0.429_{\pm 0.04} \end{array}$	$0.238_{\pm 0.06}$	$0.092_{\pm 0.01}$	$0.044_{\pm 0.02}$
Flickr	Effects	CFRNet	DRLearner	NetDeconf	G-HSIC	SPNet	CAL	Graphormer	RRNet	NetEst	CauGramer
Flickr $\epsilon_{ ext{AVE}}$	AME APE	$0.066_{\pm 0.04}$ $0.115_{\pm 0.04}$	$0.110_{\pm 0.05} \\ 0.211_{\pm 0.03}$	$0.088_{\pm 0.03}$ $0.345_{\pm 0.06}$	$0.096_{\pm 0.03}$ $0.354_{\pm 0.04}$	$0.054_{\pm 0.03}$ $0.121_{\pm 0.05}$	$0.090_{\pm 0.05}$ $0.302_{\pm 0.04}$	$\begin{array}{c} \text{Graphormer} \\ \underline{0.030}_{\pm 0.03} \\ \underline{0.409}_{\pm 0.03} \\ 0.382_{\pm 0.04} \end{array}$	$0.160_{\pm 0.03}$ $0.268_{\pm 0.09}$	$0.063_{\pm 0.04} \\ \underline{0.055}_{\pm 0.03}$	$0.028_{\pm 0.03} \\ 0.019_{\pm 0.01}$

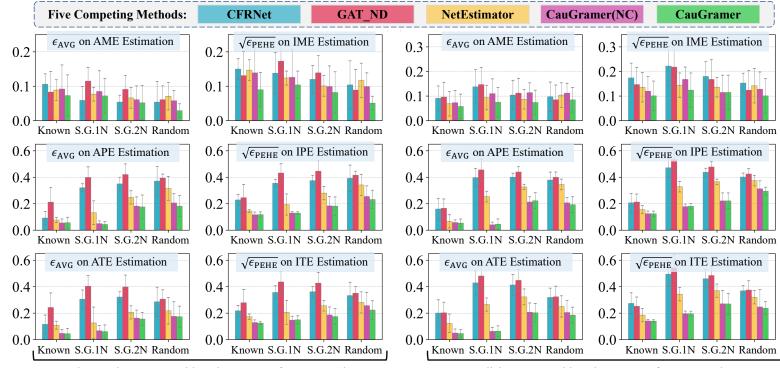
Table 3: Results of Heterogeneous Treatment Effects Estimation with/without Unconfoundedness on BlogCatalog (BC) and Flickr Datasets. The best is **boldface** while the second best is <u>underlined</u>.

BC	Effects	CFRNet	DRLearner	GDML	SPNet	NetEst	CEVAE	CNE	UNITE	C.G.(UC)	C.G.(NC)	CauGramer
$\epsilon_{ ext{AVE}}$	AME APE ATE	$\begin{array}{c} 0.106_{\pm 0.03} \\ 0.092_{\pm 0.05} \\ 0.116_{\pm 0.07} \end{array}$	$0.196_{\pm 0.07} \\ 0.183_{\pm 0.03} \\ 0.099_{\pm 0.07}$	$0.371_{\pm 0.06}$	$\begin{array}{c} 0.083_{\pm 0.06} \\ 0.212_{\pm 0.11} \\ 0.243_{\pm 0.11} \end{array}$	$0.077_{\pm 0.02}^{-}$	$\begin{array}{c} 0.081_{\pm 0.03} \\ 0.403_{\pm 0.01} \\ 0.349_{\pm 0.04} \end{array}$	$0.519_{\pm 0.05}$	-	$ \begin{vmatrix} 0.109_{\pm 0.07} \\ 0.067_{\pm 0.04} \\ 0.077_{\pm 0.05} \end{vmatrix} $	$0.055_{\pm0.03}$	$\begin{array}{c} \underline{0.073}_{\pm 0.06} \\ \underline{0.057}_{\pm 0.04} \\ 0.045_{\pm 0.04} \end{array}$
$\sqrt{\epsilon_{ ext{PEHE}}}$	IME IPE ITE	$\begin{array}{c} 0.150_{\pm 0.03} \\ 0.229_{\pm 0.04} \\ 0.218_{\pm 0.04} \end{array}$	$\begin{array}{c} 0.544_{\pm 0.03} \\ 0.216_{\pm 0.03} \\ 0.529_{\pm 0.02} \end{array}$	$0.411_{\pm 0.06}$	$\begin{array}{c} 0.131_{\pm 0.07} \\ 0.246_{\pm 0.10} \\ 0.279_{\pm 0.10} \end{array}$	$0.145_{\pm 0.01}$	$0.439_{\pm 0.01}^{-}$	$0.552_{\pm 0.05}$	0.194 _{±0.00}	$0.125_{\pm 0.02}$	$\begin{array}{c} 0.139_{\pm 0.09} \\ 0.117_{\pm 0.02} \\ \underline{0.129}_{\pm 0.02} \end{array}$	$0.090_{\pm 0.05} \\ \underline{0.118}_{\pm 0.02} \\ 0.125_{\pm 0.01}$
Flickr	Ecc.	CEDM		The state of the s								
THERE	Effects	CFRNet	DRLearner	GDML	SPNet	NetEst	CEVAE	CNE	UNITE	C.G.(UC)	C.G.(NC)	CauGramer
$\epsilon_{ ext{AVE}}$	AME APE ATE	CFRNet $0.091_{\pm 0.05}$ $0.160_{\pm 0.08}$ $0.201_{\pm 0.10}$	DRLearner $0.135_{\pm 0.08}$ $0.216_{\pm 0.02}$ $0.131_{\pm 0.07}$	$0.239_{\pm 0.08}$ $0.381_{\pm 0.02}$	$0.096_{\pm 0.06}$	$0.069_{\pm 0.05}$ $0.067_{\pm 0.05}$	$0.063_{\pm 0.04}$ $0.432_{\pm 0.05}$	$0.168_{\pm 0.05}$ $0.562_{\pm 0.06}$	$0.043_{\pm 0.00}$	` '	$0.073_{\pm 0.05} \\ \underline{0.038}_{+0.02}$	CauGramer $0.058_{\pm 0.05}$ $0.030_{\pm 0.03}$ $0.025_{\pm 0.03}$









BlogCatalog Dataset with Unknown Interference Graph

Flickr Dataset with Unknown Interference Graph

Conclusion: By constructing linear queries from individual features, graph convolutional keys from peer features, and combined values to model network interference, CauGramer expands the receptive field of the graph neural network while capturing complex interference patterns. Experiments on two widely used benchmark datasets demonstrate that the proposed CauGramer outperforms existing methods in network causal effect estimation.

Thanks

Acknowledgement

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